Elementary constraints on autocorrelation function scalings

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Abstract

Elementary algebraic constraints on the form of an autocorrelation function $C(t_w+\tau, t_w)$ rule out some two-time scalings found in the literature as possible long-time asymptotic forms. The same argument leads to the realization that two usual definitions of *many-time scale* relaxation for aging systems are not equivalent.

There are elementary model-independent constraints on the autocorrelation of an observable. For example, if an observable $A(t_1)$ is very correlated to $A(t_2)$, and $A(t_2)$ is very correlated to $A(t_3)$, it is clear that $A(t_1)$ cannot be uncorrelated from $A(t_3)$. Such kind of constraint has long been taken into account for the autocorrelations of quantities in equilibrium, but, surprisingly enough, has not been exploited in non-stationary 'aging' situations.

Consider first the case of real observable A. We can derive inequalities satisfied by the normalized autocorrelation functions

$$C_{ij} = \frac{\langle A(t_i)A(t_j)\rangle}{\sqrt{\langle A^2(t_i)\rangle\langle A^2(t_j)\rangle}} \tag{1}$$

as follows. Take arbitrary real numbers $v_1, ..., v_r$ and construct the following expectation value (throughout this paper times are adimensional):

$$\sum_{i,j=1}^{r} C_{ij} v_i v_j = \left\langle \left(\sum_{1}^{r} \frac{v_i A(t_i)}{\sqrt{\langle A^2(t_i)\rangle}} \right)^2 \right\rangle \geq 0 \qquad \forall \quad v_1, ..., v_r \tag{2}$$

This implies that any $r \times r$ matrix C_{ij} has to be nonnegative, i.e. all its eigenvalues should be nonnegative. In particular, demanding that the determinant of C_{ij} be positive we get, for any two times:

$$1 - C_{12}^2 \geq 0 \tag{3}$$

and for any three times ($r = 3$):

$$1 - C_{12}^2 - C_{23}^2 - C_{13}^2 + 2C_{12}C_{23}C_{13} \geq 0 \tag{4}$$

A simple rearrangement of this formula gives:

$$|C_{13} - C_{12}C_{23}| \leq \left(1 - C_{12}^2\right)^{1/2} \left(1 - C_{23}^2\right)^{1/2} \tag{5}$$

which, if C_{12} and C_{23} are positive implies:

$$C_{13} \geq C_{12}C_{23} - \left(1 - C_{12}^2\right)^{1/2} \left(1 - C_{23}^2\right)^{1/2} \tag{6}$$

This is the algebraic expression of the fact mentioned above: if C_{12} and C_{23} are close to one, then C_{13} is too.

Autocorrelations that arise frequently in particle systems are the coherent and incoherent functions obtained from:

$$\bar{Z}_{ij}^{coh} \equiv \left\langle \sum_a e^{i\vec{k}\cdot(\vec{x}_a(t_i) - \vec{x}_a(t_j))} \right\rangle \quad ; \quad \bar{Z}_{ij}^{inc} \equiv \left\langle \sum_{ab} e^{i\vec{k}\cdot(\vec{x}_a(t_i) - \vec{x}_b(t_j))} \right\rangle \tag{7}$$

We shall consider the normalized versions obtained from the real part of:

$$C_{ij}^{inc} \equiv \mathrm{Re}\, Z_{ij}^{coh} \quad ; \quad Z_{ij}^{coh} = Z_{ji}^{*\,coh} = \frac{\bar{Z}_{ij}^{coh}}{\sqrt{\bar{Z}_{ii}^{coh} \bar{Z}_{jj}^{coh}}} \tag{8}$$

and similarly for Z_{ij}^{inc} and C_{ij}^{inc}. The normalization for the incoherent version is constant, while for the coherent correlation it is the modulus of the equal time structure function evaluated at the wavevector $\vec{k}$.

One can obtain a constraint similar to (6):

$$C_{13}^{\mathcal{R}} \geq 1 - \mathcal{F}(C_{12}, C_{23}) \tag{9}$$

with $\mathcal{F}$ vanishing when C_{12} and C_{23} are close to one (see the Appendix for the precise form of $\mathcal{F}$ and its derivation).

Before continuing, let us point out that, because what matters in this argument are only the values of correlations and their time-orderings, we immediately conclude that if a two-time correlation function $C(\tau+t_w,t_w)$ satisfies the criteria (6) or (9), so does any time reparametrization $C(h(\tau+t_w),h(t_w))$, with any monotonic and otherwise arbitrary h. (Note that h acts on total times, rather than on time differences).

We have written the inequalities for the normalized correlations. This is slightly non-standard, although implies no modification in a stationary case, as the normalization factor is then a constant. Even in a nonstationary aging situation, if we are interested in the scaling regime in which all times are large, the normalisation becomes a constant:

$$N_\infty \equiv \lim_{t\to\infty} \langle |A(t)|^2 \rangle \tag{10}$$

a limit that in a relaxational case exists and is non-negative, since it is the expectation value of a positive operator. We shall assume that the correlation studied is such that its equal-time value N_∞ does not tend to zero at large times.

i) Conditions on the scaling variable

The simplest correlation form for an aging system is:

$$C(\tau+t_w,t_w) = \mathcal{C}_1(\tau) + qC_{aging}(\tau+t_w,t_w) \tag{11}$$

where we have set $C_{aging}(t_w,t_w)=1$ and q is the Edwards-Anderson 'nonergodicity' parameter. Perhaps the most frequently used form for $C_{aging}(\tau+t_w,t_w)$ is[1,2]:

$$C_{aging}(\tau+t_w,t_w) = \mathcal{C}_2\left(\frac{\tau}{t_w^\mu}\right) \tag{12}$$

or, more generally:

$$C_{aging}(\tau+t_w,t_w) = \mathcal{C}_2\left(\frac{\tau}{g(t_w)}\right) \tag{13}$$

To obtain g from experimental data, one computes the time $\tau^*(t_w)$ for the correlation to fall to some value C^*. This fixes $g(t_w) = \tau^*(t_w)$, but one has to check that $g(t_w)$ does not depend on the chosen value of C^*.

Let us see that *for any $g(t_w)$ growing faster than t_w (e.g. t_w^μ with $\mu > 1$) this scaling form is inconsistent*, in the sense that there can be no continuous large-t_w limit for $\mathcal{C}_2$. In particular, the fitting procedure mentioned above necessarily fails to give an unique $g(t_w)$ if taken to very long times.

We first consider the case in which the stationary part is absent ($\mathcal{C}_1(\tau) = 0$) and then show that the argument holds also for the more general form (11). Assume there is a smooth, nonincreasing scaling function $\mathcal{C}_2$. Choose three times $t_1 < t_2 < t_3$ such that $t_1 >> 1$ and $0 < C_{aging}(t_2, t_1) < 1$ and $0 < C_{aging}(t_3, t_2) < 1$. For this to be possible, the arguments in $\mathcal{C}_2$ should be non-zero and finite. If $\mu > 1$, this requires that, as $t_1 \to \infty$:

$$\frac{t_2 - t_1}{t_1^\mu} \sim \frac{t_2}{t_1^\mu} \quad \textit{and} \quad \frac{t_3 - t_2}{t_2^\mu} \sim \frac{t_3}{t_2^\mu} \tag{14}$$

should be finite numbers. Writing:

$$\frac{t_3 - t_1}{t_1^\mu} \sim \frac{t_3}{t_1^\mu} = \left(\frac{t_3}{t_2^\mu}\right)\left(\frac{t_2}{t_1^\mu}\right)^\mu \, t_1^{\mu(\mu-1)} - t_1^{-(\mu-1)} \to \infty \ , \tag{15}$$

we notice that under these circumstances $C_{aging}(t_3, t_1) \to \mathcal{C}_2(\infty)$: even though the two correlations $C_{aging}(t_2, t_1)$ and $C_{aging}(t_3, t_2)$ can be as close to one as one wishes, the third correlation $C_{aging}(t_3, t_1)$ takes the smallest possible value (usually zero). Hence, the scaling violates (6) or (9), and is hence not possible. The argument goes through for any $g(t_w)$ that grows faster than t_w.

In order to extend the reasoning to the general case (11), it suffices to note that one can replace the observables $A(t_i)$ by a smoothed set:

$$\hat{A}_\sigma(t_i) = \int_0^\infty dt' A(t') e^{(t'-t_i)^2/\sigma^2} \tag{16}$$

and run the preceding argument for the normalized correlations of the $\hat{A}_\sigma(t_i)$. It is easy to check that for large σ, the stationary part is ironed out, and the form (11) reduces to the

one assumed in the previous paragraph. One can also check that a finite sum of terms (13) with some $g(t_w)$ growing faster than t_w still lead to impossible asymptotic scalings.

ii) **Conditions on the scaling function.**

We have shown that there are two-time scaling variables that are impossible as asymptotic scaling forms - whatever the form of the scaling function $\mathcal{C}_2$. Other scaling variables are in principle legitimate, although there are in those cases conditions on the scaling function. Consider the stationary case, in which correlations depend on time-differences:

$$C(\tau + t_w, t_w) = \mathcal{C}_1(|\tau|) \tag{17}$$

Then,

$$\int dt' \mathcal{C}_1(|t - t'|) e^{i\omega t'} dt' = \hat{C}(\omega) e^{i\omega t} \tag{18}$$

says that the Fourier components $\hat{C}(\omega)$ are the eigenvalues, and the condition of positivity becomes the positivity condition on the Fourier components $\hat{C}(\omega)$. A similar condition can be found for the domain-growth correlation form:

$$C_{aging}(\tau + t_w, t_w) = \mathcal{C}_2\left(\frac{L(t_w)}{L(t_w + \tau)}\right) \qquad \text{for} \qquad \tau \geq 0 \tag{19}$$

with some monotonically increasing function $L(t)$. Writing:

$$C_{aging}(\tau + t_w, t_w) = \mathcal{C}_2\left[e^{|\ln L(t_w) - \ln L(t_w+\tau)|}\right] \tag{20}$$

we realize that we are back in the stationary case, with this time a scaling function $\tilde{\mathcal{C}}(x) \equiv \mathcal{C}_2(e^x)$, and the time-reparametrization $h(t) = \ln(L(t))$. Furthermore, because the addition of two positive operators is a positive operator, we conclude that the additive form:

$$C(\tau + t_w, t_w) = \mathcal{C}_1(|\tau|) + q\mathcal{C}_2\left(\frac{L(t_w)}{L(t_w + \tau)}\right) \tag{21}$$

is admissible if each term is admissible separately.

iii) Superaging.

Consider a correlation having scaling form:

$$C(\tau + t_w, t_w) = \mathcal{C}\left(\frac{\ln t_w}{\ln(\tau + t_w)}\right) \tag{22}$$

where the times are adimensional. The scaling happens in several real systems, it corresponds for example to logarithmic domain growth[4]. It is an example of a 'superaging'[5] situation (i.e., one where the scaling function $L(t)$ in the form (19) grows slower than a power of time).

Let us show that:

$$\mathcal{C}\left(\frac{\ln t_w}{\ln(\tau + t_w)}\right) \sim \int_1^\infty d\mu\ \rho(\mu) \exp\left(-\frac{\tau}{t_w^\mu}\right) \quad \text{with} \quad \rho(\mu) = -\frac{d}{d\mu}\mathcal{C}\left(\frac{1}{\mu}\right) \tag{23}$$

Put $x \equiv \frac{\ln \tau}{\ln t_w}$. For $t_w \to \infty$, we have that $\frac{\ln t_w}{\ln(\tau+t_w)} \sim 1/x$ for $x > 1$, and $\frac{\ln t_w}{\ln(\tau+t_w)} \sim 1$ for $x \leq 1$. Hence:

$$\int_1^\infty d\mu\ \rho(\mu) \exp\left(-\frac{\tau}{t_w^\mu}\right) = \int_1^\infty d\mu\ \rho(\mu) \exp\left(-t_w^{(x-\mu)}\right) \sim \int_1^\infty d\mu\ \rho(\mu)\Theta(\mu - x) \tag{24}$$

where Θ is the step function. The last relation becomes exact in the limit of large t_w. The integral for $x \leq 1$ yields 1, and for $x > 1$:

$$\int_x^\infty d\mu\ \rho(\mu) = \mathcal{C}\left(\frac{1}{x}\right) \tag{25}$$

where we have used the form of ρ in (23).

Equation (23) shows that one obtains an admissible correlation functions as a superposition of infinitely many terms of the form (12) having $\mu > 1$.

iv) Many time scales.

The distinction between aging systems having two or more than two time-scales is of importance since it helps distinguishing the underlying physics. Indeed, the absence of many timescales in spin glass dynamics is a strong obstacle for the identification of realistic

systems with their mean-field counterpart[2,6]. Under these circumstances, it is important to point out that two definitions of 'many timescales' found in the literature are inequivalent.

Consider the following definition of time scale:

Def.1 : If a correlation is a sum of terms of the form $\mathcal{C}_\alpha(\tau/g_\alpha(t_w))$, with each $g_\alpha(t_w)$ growing at a different rate, then each such term defines a different time-scale. With this definition the logarithmic domain-growth law (22) has infinitely many time scales, as we see from equation (23).

A different definition that arises naturally in the construction of the analytic solution of the aging dynamics of glass models[3,2] is the following:

Def.2 : Two correlation values c and c^* belong to the same time scale if, given that $C(t_2,t_1) = c$ and $C(t_3,t_2) = c^*$, then $C(t_3,t_1)$ stays smaller than $\min(c,c^*)$ in the large times limit.

Now, it is easy to check that with this definition the scaling (22) consists of a single time scale, and it can be taken by the reparametrization $t \to h(t)$ to the simple aging form. We conclude that, depending on the definition of 'time scale', we have in this case one or infinitely many slow time scales! Hence, we have shown that definitions 1 and 2 are not in general equivalent.

The reason why Definition 2 is the natural one for the analytic treatment[3,2] is that this way of introducing time scales is insensitive to time-reparametrizations $t \to h(t)$, since times enter only through their ordering. This is not the case of Definition 1, under which a one-time scale dependence $\frac{t_w}{\tau+t_w}$ becomes an infinite-time scale dependence upon reparametrization $t \to \ln t$. Physically, robustness with respect to time-reparametrizations is a relevant feature of a characterization of slow dynamics since in such systems a very weak perturbation can have the effect of time-reparametrising the aging part of the correlations and responses. The most clear examples of this are the growth law of domains in coarsening systems – which is taken from power law to logarithmic by an arbitrarily weak pinning field, and the effect of shear in soft glasses, which eliminates aging altogether.

In conclusion, we have emphasized that a two-time scaling is not a generic function of

two variables, but has limitations that become manifest when one considers three successive times.

I. APPENDIX

Taking arbitrary complex numbers $v_1, ..., v_r$ it is easy to show that, just as in the real case, both for the coherent and for the incoherent function:

$$\sum_{i,j=1}^{r} Z_{ij} v_i^* v_j \geq 0 \qquad \forall \quad v_1, ..., v_r \tag{26}$$

This implies that all the eigenvalues of any $r \times r$ matrix Z_{ij} are nonnegative. (We have dropped the label *inc* and *coh*, as the derivation applies to both).

Let us obtain a bound (9). Demanding that the determinant of a three by three matrix be positive, we have:

$$1 - |Z_{12}|^2 - |Z_{23}|^2 - |Z_{13}|^2 + Z_{12} Z_{23} Z_{13}^* + Z_{12}^* Z_{23}^* Z_{13} \geq 0 \tag{27}$$

Rearranging terms:

$$\left(1 - |Z_{12}|^2\right)\left(1 - |Z_{23}|^2\right) \geq |Z_{13} - Z_{12} Z_{23}|^2 \tag{28}$$

Put $D_{ij} \equiv (1 - Z_{ij})$. Then, (28) reads:

$$\left(1 - |Z_{12}|^2\right)\left(1 - |Z_{23}|^2\right) \geq |D_{13} - D_{12} - D_{23} + D_{12} D_{23}|^2 \tag{29}$$

Applying the inequality $|a| \leq |a - b| + |b|$ to (29) we obtain:

$$|D_{13}| \leq |D_{13} - D_{12} - D_{23} + D_{12} D_{23}| + |D_{12} + D_{23} - D_{12} D_{23}| \tag{30}$$

which, inserting (29) implies:

$$|D_{13}| \leq \left(1 - |Z_{12}|^2\right)^{1/2}\left(1 - |Z_{23}|^2\right)^{1/2} + |D_{12} + D_{23} - D_{12} D_{23}| \tag{31}$$

We can express this bound exclusively in terms of C_{12} and C_{23}. First, note that:

$$\left(1-|Z_{ij}|^2\right) \leq \left(1-|C_{ij}|^2\right) \tag{32}$$

since addition of the square of the imaginary part can only make the bracket larger. We also have:

$$|D_{ij}|^2 = |1-Z_{ij}|^2 = 1-2C_{ij}+|Z_{ij}|^2 = 2\left(1-C_{ij}\right) - \left(1-|Z_{ij}|^2\right) \leq 2\left(1-C_{ij}\right) \tag{33}$$

where we have used that $|Z_{ij}|^2 < 1$. Inserting these two last inequalities in (31), we get:

$$|1-Z_{13}| \leq \mathcal{F} \tag{34}$$

with:

$$\begin{aligned} \mathcal{F} \equiv & \left(1-|C_{12}|^2\right)^{1/2}\left(1-|C_{23}|^2\right)^{1/2} + \sqrt{2}|1-C_{12}|^{1/2} + \sqrt{2}|1-C_{23}|^{1/2} \\ & + 2|1-C_{12}|^{1/2}|1-C_{23}|^{1/2} \end{aligned} \tag{35}$$

Z lies within a circle of radius $\mathcal{F}$ in the complex plane centered in one, hence we get:

$$C_{13} \geq 1-\mathcal{F} \tag{36}$$

We can see that when C_{12} and C_{23} are closed to unity, C_{13} cannot be small. Perhaps a better or simpler bound can be obtained, but this is enough for the present purposes.

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